The Challenge and Promise of Scientific Computing

Summary

The U.S. faces a major challenge in scientific computing, one of the foundations of scientific discovery in the 21st century. A clear path is available for the U.S. to sustain leadership in this critical field.

Recently, with the start-up of its new supercomputer, known as the Earth Simulator, the Japanese introduced the world to a new era in scientific computation. The Earth Simulator is an impressive machine. It has the computing power of the 20 fastest U.S. computers combined and a peak speed of 40 teraflops—three times faster than the theoretical peak performance of any U.S. machine. Initially designed for climate change studies, the Earth Simulator has applications across a broad range of scientific problems from the geosciences to fusion.

In the next few years, we expect the Japanese to build on their success with the Earth Simulator to develop other, more powerful general-purpose computers. Their strategy seems clear: to provide a focused ultra-high-end computing resource, recruit the best and brightest scientists to collaborate on its use, acquire the knowledge needed to dominate a computational science discipline, and develop the computer codes to harness that knowledge. The U.S Department of Energy's Office of Science understands this strategy very well because it is the one we developed and used to lead the world in the areas of computational science that are important to DOE's missions.

In the last decade, the power of computation—our ability to model and simulate experiments that we have not conducted in a laboratory—has become so great that it must now be considered a third pillar, along with theory and experiment, in the triad of tools used for scientific discovery. This means, in effect, that computing power will increasingly be the limiting factor in many areas of scientific endeavor. What's more, it will only become more critical as computing power becomes key to scientific leadership in many fields. As the Japanese clearly recognize, more efficient and more powerful computers are essential to fueling the pace of scientific discovery—and the solutions to many of our most pressing national and international challenges.

Computational science capabilities already underpin the research and development that DOE conducts to meet its energy and national security missions. Because these capabilities are central to DOE's missions, and because computational capability is also so critical to scientific discovery generally, it is appropriate that DOE's Office of Science brings a renewed focus to this challenge.

The Office of Science's Role

The Office of Science has been the world leader in using advanced computers for scientific discovery for the past 50 years. We have a strong tradition of working closely with computer vendors to bring their high-end machines into productive use. In collaboration with other federal agencies and the academic community, we have provided both intellectual and technological leadership for this national effort. Beginning more than 25 years ago, the Office of Science deployed supercomputing capability in the Magnetic Fusion Energy Computing Center, which has since evolved into the National Energy Research Scientific Computing Center (NERSC), a successful model that the National Science Foundation in turn adopted with their supercomputer centers.

Today, Office of Science research programs in Biological and Environmental Research, Basic Energy Sciences, High Energy and Nuclear Physics, and Fusion Energy Sciences all are exploiting supercomputing. To further this trend, the Scientific Discovery through Advanced Computing (SciDAC) program was initiated in FY 2001, and it is now bringing advanced computation to bear on fundamental problems throughout the sciences.

The national research community's need for scientific computing capability is huge—even before the SciDAC program was launched, the Office of Science was able to satisfy only a third of the demand for high-performance computing. The U.S. scientific community suffers both from the lack of computing capacity and the lack of computing capability—the ability to perform the largest simulations. The Office of Science has a clear role to play in filling this gap.

The Approach

The Earth Simulator is an extraordinarily well-integrated machine based on conventional technology. However, new technologies on the horizon promise to make the power of an Earth Simulator far cheaper and easier to realize. One such technology is the "processor in memory" architecture that involves the integration of a microprocessor and associated memory on a single silicon chip. Another is the optical interconnect—which replaces the thousands of miles of copper wire in a conventional computer with ultra-high-bandwidth fiber connections. Together, such technologies lead many scientists to believe that a petaflop computer, one with 25 times the capability of the Earth Simulator, is within reach. By spearheading an effort to develop such technologies, the Office of Science has the opportunity to lead the coming scientific computing revolution. The following steps provide a pathway to delivering U.S. scientists the computing power they need:

- A strong partnership between the Office of Science and computer vendors must be reinvigorated to drive the development of promising computing architectures for science simulations.

- In the short term, the science gap in the U.S. created by the Earth Simulator can be reduced by significantly enhancing existing high-end computing capability and networking.

- In the mid and long term, an aggressive, integrated portfolio of investments in advanced architecture, computational science, and focused technology deployment will dramatically advance the nation's science mission and allow the U.S. to regain and sustain the lead in supercomputing and its applications.

- Focused collaborations with other Federal agencies and the academic community will foster the development of the best computational science to exploit these new capabilities. The Office of Science will build on the success of SciDAC by promoting innovative partnerships between applied mathematicians, computer scientists, computational scientists, and other disciplines to apply ultra-scale computation to problems of national interest and priority.

The Office of Science believes that the opportunities made available by the revolution in scientific computation, foreshadowed so clearly by the Earth Simulator, will lead to extraordinary new scientific capabilities for the Nation. We must build and strengthen the third pillar of the triad of discovery if we are to probe the deepest secrets of Nature and reap the technical, economic, and social benefits such understanding will yield.

For further information on this subject contact:
Dr. Edward Oliver, Director
Office of Advance Scientific Computing Research
301-903-7486
Ed.Oliver@science.doe.gov